Ex (2): Find the Constants of the functions $\psi_1 = Ae^{-ix}$

$\psi_2 = B\sin(ax)$, in the region $[0, a]$, and which one is an eigenfunction Corresponding to P_x, P_x^2, T.

Solution

1- Find the Constant in the region $[0, a]$

The Process of normalization:

$$N\psi(x,t) \longrightarrow \int_{-\infty}^{\infty} N^* \psi^* N \psi \, dx = 1 \quad \therefore |N|^2 \int_{-\infty}^{\infty} \psi^* \psi \, dx = 1$$

$\therefore \psi_1 = Ae^{-ix}$, by applying the normalization process:

$$\therefore \int A^* \psi_1^* A \psi_1 = 1 \quad \therefore A^2 \int e^{-dx} e^{ix} \, dx = 1$$

$$\therefore A^2 \int_0^a dx = 1 \quad \therefore A^2 a = 1 \quad \therefore A = \frac{1}{\sqrt{a}} \text{ Constant of } \psi_1$$

$$\therefore \psi_1 = \frac{e^{-ix}}{\sqrt{a}} .$$

$\therefore \psi_2 = B\sin(ax)$, first find a, by applying the boundry Conditions $[0, a]$

$$\psi_2(0) = \psi_2(a) = 0$$

$\therefore B\sin(\quad) = 0 \quad , \therefore B \neq 0 \quad \therefore \sin(\quad) = 0$

$\therefore \alpha a = n\pi \quad \therefore \alpha = \frac{n\pi}{a}$

$\therefore \psi_2 = B \sin\left(\frac{n\pi}{a}\right)$, by applying the normalization process

$\therefore \int_0^a B^* \psi_2^* B \psi_2 \, dx = 1$

$\therefore B^2 \int_0^a \sin\left(\frac{n\pi x}{a}\right) \sin\left(\frac{n\pi x}{a}\right) dx = 1 \quad \therefore B^2 \int_0^a \sin^2\left(\frac{n\pi x}{a}\right) dx = 1$

$\therefore \cos(2\theta) = 1 - 2\sin^2\theta$

$\therefore B^2 \int_0^a \sin^2\left(\frac{n\pi x}{a}\right) dx = \frac{B^2}{2} \int_0^a \left[1 - \cos\left(\frac{2n\pi x}{a}\right)\right] dx = 1$

$\therefore \frac{B^2}{2} \int_0^a dx = 1 \quad \therefore \frac{B^2}{2} \cdot a = 1 \quad \therefore B = \sqrt{\frac{2}{a}}$

$\therefore \psi_2 = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$

2- Eigenfunctions

Lecture (3) 5/7/2026

One Dimensional Problems

Infinite square well , step Potential $E > V$

The application of the Schrödinger equation to one-dimensional problems enable us to compare the predictions of classical and quantum mechanics in a simple setting.

The Schrödinger equation describing the dynamics of a microscopic particle of mass m in a 1-D time-independent potential $V(x)$ is given by

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

where:

E: is the total energy of the particle.

The solutions of this equation yield the allowed energy eigenvalues E_n corresponding wavefunction $\psi_n(x)$

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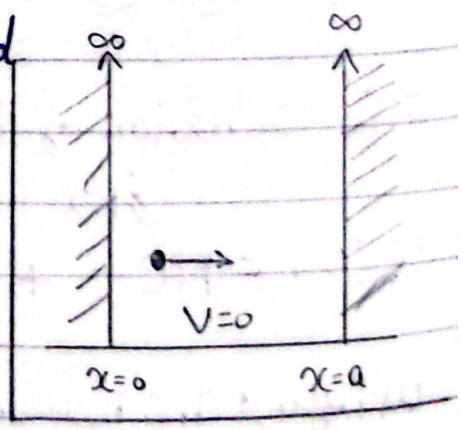
1 - The infinite square well Potential: الجسيم الحر داخل البئر الكمي

Considre a particle of mass m confined to move inside an infinitely deep assymetric potential well

$$V(x) = \begin{cases} +\infty & x<0 \\ 0 & 0<x<a \\ +\infty & x>a \end{cases}$$



Solution of This Problem

The Time independent Schrödinger equation (TISE):

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x)$$

Since outside the boundries the Potential $V(x) = \infty$ Then the wave function of the Particle must be zero outside the boundary. Hence we will look for solutions only inside the well.

Inside the well : $V(x) = 0$; means that the Particle moves freely, and then TISE be

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \quad \therefore \quad \frac{-d^2\psi}{dx^2} = \frac{2mE}{\hbar^2}\psi$$

$$\therefore \frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0 \quad (1), \quad \because E = \frac{p^2}{2m} \therefore p^2 = 2mE$$

$$, \because p = \hbar k \quad \therefore p^2 = \hbar^2 k^2 = 2mE \quad \therefore \frac{2mE}{\hbar^2} = k^2 \quad (2)$$

Sub. from (2) in (1) $\therefore \frac{d^2\psi}{dx^2} + k^2\psi = 0$

The solution of this DE is known

$$\psi(x) = Ae^{ikx} + Be^{-ikx} = A\sin(kx) + B\cos(kx)$$

applying the boundary Conditions

1- $\psi(x=0)=0$

$\therefore 0 = A\sin(0) + B\cos(0)$ $\quad \therefore B = 0$

$\therefore \psi(x) = A\sin(kx)$

2- $\psi(x=a)=0$

$\therefore 0 = A\sin(ka)$ $\quad \therefore \sin(ka)=0$ $\quad \therefore ka = n\pi$

$\therefore k^2a^2 = n^2\pi^2$ $\quad , k^2 = \frac{2mE}{\hbar^2}$

$\therefore \frac{2mE}{\hbar^2}a^2 = n^2\pi^2$ $\quad \therefore \boxed{E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}}$

E_n : is the total energy of the particle in the system, and it takes discrete values, the particle can exist only in these certian allowed energy levels. E_n is called 'Eigenvalue'.

to find the constant A, we need to normalize the wave function $\psi(x)$:

$$\int_{-\infty}^{\infty} A\sin(kx)\cdot A\sin(kx)\,dx = 1$$

$$\therefore |A|^2 \int_{-\infty}^{\infty} \sin^2(kx)\,dx = 1$$

The Particle can only be found in the region $[0, a]$, Then the normalization goes to:

$$|A|^2 \int_0^a \sin^2(kx)\,dx = 1 \quad , \because \cos(2\theta) = 1 - 2\sin^2\theta$$

$$\therefore \sin^2\theta = \frac{1}{2}\left[1 - \cos(2\theta)\right]$$

$$\therefore |A|^2 \cdot \frac{1}{2} \int_0^a (1 - \cos(2kx))\,dx = 1$$

$$\therefore \frac{1}{2}|A|^2 \left[\int_0^a dx - \int_0^a \cos(2kx)\,dx\right] = 1$$

$$\therefore \frac{1}{2}|A|^2 \left[a - \frac{1}{2k}\sin(2kx)\Big|_0^a\right] = 1$$

$\because k = \frac{n\pi}{a}$ ⇒

$$\therefore \frac{1}{2}|A|^2 \left[a - \frac{1}{2k}\sin\left(\frac{2n\pi x}{a}\right)\Big|_0^a\right] = 1$$

(goes to zero)

$$\therefore \frac{1}{2}|A|^2 a = 1 \quad \therefore A = \sqrt{\frac{2}{a}}$$

Then

$$\boxed{\psi(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)}$$ ← The Eigenfunction

↳ $n = 1, 2, 3, \ldots$

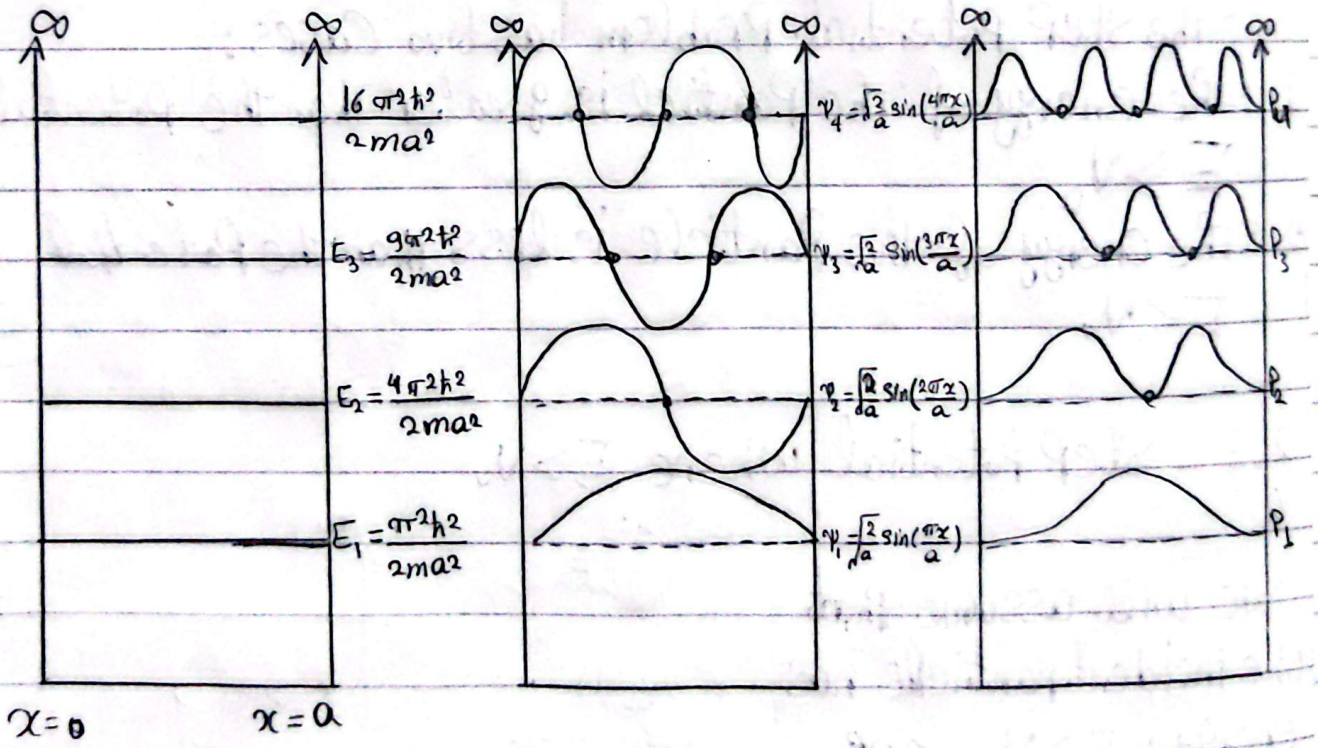
∴ Time dependent SE : $\psi_n(x,t) = \psi(x)\, e^{-i\frac{E_n}{\hbar}t}$

∴ $$\boxed{\psi_n(x,t) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) e^{-i(E/\hbar)t}}$$

2- Probability Density :

$$P_n = |\psi_n(x,t)|^2 = \frac{2}{a}\sin^2\left(\frac{n\pi x}{a}\right)$$ لا يعتمد على $e^{-iE/\hbar t}$

3- Representation of the energy, eigenfunction, and Probability density.



There are some points inside the potential well, has zero probability of finding the particle, these points are the nodes.

2- The Potential Step: (جهد السلم)

The Potential Step is one of the most fundamental Problems in 1-D Quantum mechanics. It describes a situation where a Particle moves through a region and encounters a sudden, Instantaneous change in its Potential energy (V) at a Specific Point.

What is Potential? It's a term in schrödinger equation that guides the movement of a Quantum Particle. Like, bias, barrier, energy due to Position.

الكترون عايز ينتقل من معدن إلى فراغ أو من مادة موصلة إلى عازلة فيواجه عائق مفاجئ نمثله هنا بجهد السلم (Step Potential)

The step Potential Problem has two Cases:

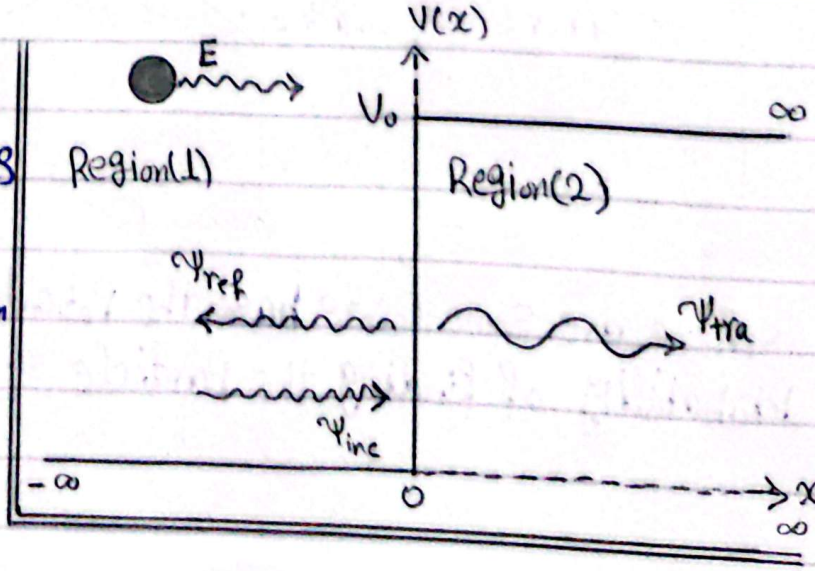
1- The energy of The Pantiel is greater Than the Potential $E > V_0$

2- The energy of the Particle is less than the Potential $E < V_0$

2.1 - Step Potential where $E > V_0$

We will assume that the incident Particle has energy: $E > V_0$, is coming from infinty from the left. where

$$V(x) = \begin{cases} 0 \; ; x < 0 \\ V_0 \; ; x > 0 \end{cases}$$



We will find the eigenfunctions, Reflection Probability and Transmission probability (coefficient).

We want to solve TISE in Regions ① and ②

In Region (1), suppose the solution is ψ_1.

the TISE is

$$\frac{-\hbar^2}{2m}\frac{d^2\psi_1}{dx} + V(x)\psi_1 = E\psi_1 \quad \text{, but } V(x)=0 \text{ in R(1)}$$

$$\therefore \frac{-\hbar^2}{2m}\frac{d^2\psi_1}{dx} = E\psi_1 \qquad \therefore \frac{d^2\psi_1}{dx} + \frac{2mE}{\hbar^2}\psi_1 = 0$$

$$\therefore \frac{d^2\psi_1}{dx} + k_1^2\psi_1 = 0 \longrightarrow \text{This DE has a standard solution}$$

$$\therefore \psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$$

The 1st term represents a wave moving in the Positive x-direction

The 2nd term represents a wave moving in the negative x-direction

$$\therefore \boxed{\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x} = \psi_{inc} + \psi_{ref}}$$

ψ_{inc} : forward moving incident wave, ψ_{ref} : Backward moving reflected wave.

In Region (2) suppose the solution is ψ_2.

the TISE

$$\frac{-\hbar^2}{2m}\frac{d^2\psi_2}{dx} + V(x)\psi_2 = E\psi_2 \quad \text{, but } V(x)=V_0 \text{ in R(2)}$$

$$\therefore \frac{d^2\psi_2}{dx} + \frac{2m}{\hbar^2}(E-V_0)\psi_2 = 0$$

$\therefore \frac{d\psi_2}{dx} + k_2^2 \psi_2 = 0 \longrightarrow$ Standard DE

$\therefore \psi_2(x) = Ce^{ik_2x} + De^{-ik_2x}$

The 1st term represents a transmitted wave, The 2nd term represents reflected wave.

• عشان الموجة تنعكس لازم تواجه تغير مفاجئ، لكن الجهد عند $x>0$ ممتد إلى ما لا نهاية بقيمة V_0 الثابتة بالتالي لا يمكن أن تنعكس الموجة. ①

• لا يوجد جسيمات تنتشر من اليمين الى اليسار فقط من اليسار إلى اليمين، وبالتالي لا يوجد موجة تتحرك من اليمين الى اليسار. ②

من ① ، ② الجزء الذي يمثل موجة منعكسة مرفوض

It Can not exist a reflected wave in $x>0 \rightarrow D=0$

$\therefore \psi_2(x) = Ce^{ik_2x}$ $\therefore$ $\boxed{\psi_2(x) = Ce^{ik_2x} = \psi_{tra}}$

There are two equations that Constrain (تقيد) our Coefficients A, B, and C : both the wavefunction and it derivative must be Continous at $x=0$. With these Conditions we Can Solve for B, and C in terms of A. $\rightarrow$ Boundary Conditions

1- $\psi(x)$ must be Continous at $(x=0)$.

$\therefore \psi_1(x=0) = \psi_2(x=0)$ $\therefore Ae^0 + Be^0 = Ce^0$

$\therefore A + B = C$ ①

2- $\psi'(x)$ must be Continous at $(x=0)$

$$\therefore \left.\frac{d\psi_1}{dx}\right|_{x=0} = \left.\frac{d\psi_2}{dx}\right|_{x=0}$$

$$\therefore ik_1Ae^{0} - ik_1Be^{0} = ik_2Ce^{0} \quad \therefore ik_1(A-B) = ik_2C$$

$$\therefore A-B = \frac{k_2}{k_1}C \quad (2)$$

by adding (1) to (2):

$$A+B+A-B = C+\frac{k_2}{k_1}C = C\left(1+\frac{k_2}{k_1}\right)$$

$$\therefore 2A = \left(\frac{k_1+k_2}{k_1}\right)C \quad \therefore \boxed{\frac{C}{A} = \frac{2k_1}{k_1+k_2}} \quad (3)$$

$$\therefore C = \left(\frac{2k_1}{k_1+k_2}\right)A \rightarrow \text{substitute in (1)}$$

$$\therefore A+B = \left(\frac{2k_1}{k_1+k_2}\right)A \quad \therefore B = A\left(\frac{2k_1}{k_1+k_2}-1\right)$$

$$\therefore \boxed{\frac{B}{A} = \frac{k_1-k_2}{k_1+k_2}} \quad (4)$$

$$\therefore k_1^2 = \frac{2mE}{\hbar^2}, \; k_2^2 = \frac{2m}{\hbar^2}(E-V_0) \quad \therefore \frac{k_2^2}{k_1^2} = \frac{E-V_0}{E}$$

$$\therefore \frac{k_2^2}{k_1^2} = 1-\frac{V_0}{E} \quad \therefore \boxed{\frac{k_2}{k_1} = \sqrt{1-\frac{V_0}{E}}} \quad (5)$$

Right now we want to find the Probability of reflection and Transmission.

Reflection Coefficient : $R = \left| \frac{\text{Reflected current density}}{\text{Incident current density}} \right|$

$$R = \left| \frac{J_{ref}}{J_{inc}} \right|$$

Transimssion Coefficient : $T = \left| \frac{\text{Transmitted current density}}{\text{Incident current density}} \right|$

$$T = \left| \frac{J_{tra}}{J_{inc}} \right|$$

Probability current density : $J = \frac{-i\hbar}{2m}\left(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx}\right)$

So to evaluate R,T we need to find J_{ref} , J_{TRA} , J_{inc} .

$\therefore \psi_{inc} = Ae^{ik_1x} \longrightarrow \psi^*_{inc} = A^* e^{-ik_1x}$ (ψ مرافق ψ^*)

$\therefore \psi_{ref} = Be^{-ik_1x} \longrightarrow \psi^*_{ref} = B^* e^{ik_1x}$

$\therefore \psi_{tra} = Ce^{ik_2x} \longrightarrow \psi^*_{tra} = C^* e^{-ik_2x}$

$AA^* = |A|^2$

$$\therefore J_{inc} = \frac{-i\hbar}{2m}\left(A^* e^{-ik_1x} \cdot ik_1 A e^{ik_1x} - Ae^{ik_1x} \cdot -ik_1 A^* e^{-ik_1x}\right)$$

$$\therefore J_{inc} = \frac{-i\hbar}{2m}\left(ik_1|A|^2 + ik_1|A|^2\right) = \frac{-i\hbar}{2m}(ik_1)(2|A|^2)$$

$$\therefore J_{inc} = \frac{\hbar k_1}{m}|A^2| \quad \therefore \boxed{J_{inc} = |A|^2 \frac{\hbar k_1}{m}} \quad (6)$$

2- $J_{ref} = \frac{-i\hbar}{2m}\left(\psi^*_{ref}\frac{d\psi_{ref}}{dx} - \psi_{ref}\frac{d\psi^*_{ref}}{dx}\right)$

$\therefore J_{ref} = \frac{-i\hbar}{2m}\left(B^* e^{ik_1x}(-ik_1B)e^{-ik_1x} - Be^{-ik_1x}\cdot ik_1Be^{ik_1x}\right)$

$\therefore J_{ref} = \frac{-i\hbar}{2m}\left(-ik_1|B|^2 - ik_1|B|^2\right) = \frac{-i\hbar}{2m}(-2ik_1|B|^2)$

$\therefore \boxed{J_{ref} = \frac{-\hbar k_1}{m}|B|^2}$ (7)

3- $J_{tra} = \frac{-i\hbar}{2m}\left(\psi^*_{tra}\frac{d\psi_{tra}}{dx} - \psi_{tra}\frac{d\psi^*_{tra}}{dx}\right)$

$\therefore J_{tra} = \frac{-i\hbar}{2m}\left(C^* e^{-ik_2x}\cdot ik_2Ce^{ik_2x} - Ce^{ik_2x}\cdot(-ik_2)C^*e^{-ik_2x}\right)$

$\therefore J_{tra} = \frac{-i\hbar}{2m}\left(ik_2|C|^2 + ik_2|C|^2\right) = \frac{-i\hbar}{2m}(2ik_2|C|^2)$

$\therefore \boxed{J_{tra} = \frac{\hbar k_2}{m}|C|^2}$ (8)

$\therefore R = \left|\frac{J_{ref}}{J_{inc}}\right| = \left|\frac{-\hbar k_1}{m}|B|^2 * \frac{m}{\hbar k_1}\frac{1}{|A|^2}\right| = \left|\frac{B}{A}\right|^2$

from (4) $\frac{k_1-k_2}{k_1+k_2} = \frac{B}{A}$

$\therefore R = \left|\frac{k_1-k_2}{k_1+k_2}\right|^2$: take k_1 Common factor from $\frac{k_1}{k_2}$

$\therefore R = \left|\frac{1-\frac{k_2}{k_1}}{1+\frac{k_2}{k_1}}\right|^2$, from (5) : $\frac{k_2}{k_1} = \sqrt{1-\frac{V_0}{E}}$

$\therefore R = \left(\frac{1 - \sqrt{1 - V_0/E}}{1 + \sqrt{1 - V_0/E}} \right)^2$ Reflection Coefficient.

$\therefore T = \left| \frac{J_{tra}}{J_{inc}} \right| = \left| \frac{\hbar K_2}{m} |C|^2 * \frac{m}{\hbar K_1} \frac{1}{|A|^2} \right|$

$\therefore T = \frac{K_2}{K_1} \left| \frac{C}{A} \right|^2$

from (3) : $\frac{C}{A} = \frac{2K_1}{K_1 + K_2}$, from (5) : $\frac{K_2}{K_1} = \sqrt{1 - \frac{V_0}{E}}$

$\therefore T = \sqrt{1 - V_0/E} \left(\frac{2K_1}{K_1 + K_2} \right)^2 = 4\sqrt{1 - V_0/E} \left(\frac{K_1}{K_1 + K_2} \right)$

$\therefore T = 4\sqrt{1 - V_0/E} \left(\frac{1}{1 + \frac{K_2}{K_1}} \right) = 4\sqrt{1 - V_0/E} \left(\frac{1}{1 + \sqrt{1 - V_0/E}} \right)^2$

$\therefore T = \frac{4\sqrt{1 - V_0/E}}{\left(1 + \sqrt{1 - V_0/E}\right)^2}$ Transmission Coefficient

$\therefore \psi(x) = \begin{cases} \psi_1(x) = Ae^{iK_1x} + Be^{-iK_1x} & \text{for } x < 0 \\ \psi_2(x) = Ce^{iK_2x} & \text{for } x > 0 \end{cases}$

→ The Eigen Function

$R = \left(\frac{1 - \sqrt{1 - V_0/E}}{1 + \sqrt{1 - V_0/E}} \right)^2$ → Reflection

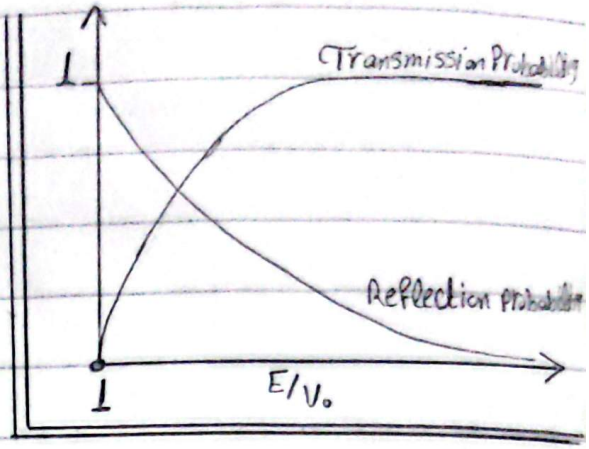
$T = \frac{4\sqrt{1 - V_0/E}}{\left(1 + \sqrt{1 - V_0/E}\right)^2}$ → Transimission

Notes:

1- $T+R=1$

2- $E \simeq V_0$, $R=1, T=0$

3- $E \gg V_0$, $R \simeq 0$, $T=1$



3- The Potential Barrier and well:

Considre a beam of Particles of mass m that are sent from left on a Potential barrier

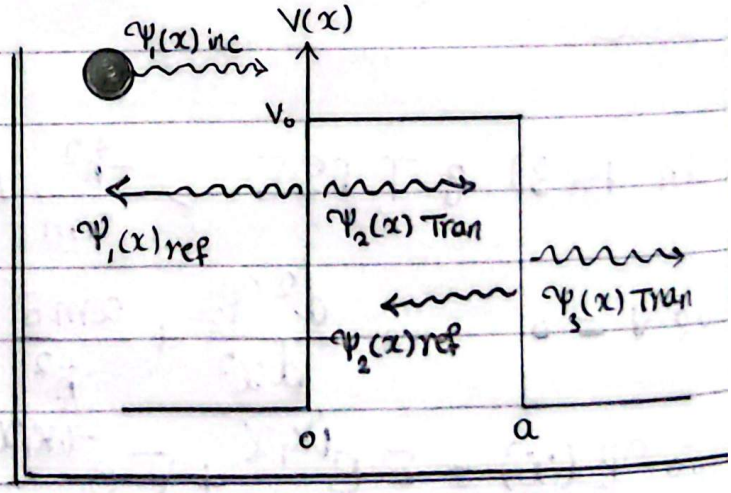
$$V(x) = \begin{cases} 0 & ; x<0 \\ V_0 & ; 0 \leq x \leq a \\ 0 & ; x>a \end{cases}$$

There are two cases, when the energy of the Particles greater than the Potential ($E>V_0$), and when the energy is less than the Potential ($E<V_0$)

3.1- The Case $E>V_0$ الدكتور مسميها التأثير النفقي

Quantum Transmission and Reflection:

we want to solve TISE in These three regions.



In R(1):

$$\frac{-\hbar^2}{2m}\frac{d^2\psi_1}{dx^2} + V(x)\psi_1 = E\psi_1$$

, $V=0$

$$\therefore \frac{-\hbar^2}{2m}\frac{d^2\psi_1}{dx^2} = E\psi_1 \qquad \therefore \frac{d^2\psi_1}{dx^2} + \frac{2mE}{\hbar^2}\psi_1 = 0$$

$$\therefore \frac{d^2\psi_1}{dx^2} + K_1\psi_1 = 0$$

$\therefore \psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x} = \psi_{inc} + \psi_{ref}$

1st term represents incident wave. 2nd term represents reflected wave

In R(2) : TISE $\rightarrow \frac{-\hbar^2}{2m}\frac{d^2\psi_2}{dx^2} + V\psi_2 = E\psi_2$

, $V = V_0$ $\therefore \frac{-\hbar^2}{2m}\frac{d^2\psi_2}{dx^2} + V_0\psi_2 = E\psi_2$

$\therefore \frac{-\hbar^2}{2m}\frac{d^2\psi_2}{dx^2} = (E - V_0)\psi_2$

$\therefore \frac{d^2\psi_2}{dx^2} - \frac{2m}{\hbar^2}(E - V_0)\psi_2 = 0$

$\therefore \psi_2(x) = Ce^{ik_2x} + De^{-ik_2x}$, $k_2^2 = \frac{2m(E - V_0)}{\hbar^2}$

1st term represents Transmitt wave, 2nd term represents reflected wave

In R(3) : TISE $\rightarrow \frac{-\hbar^2}{2m}\frac{d^2\psi_3}{dx^2} + V\psi_3 = E\psi_3$

$\therefore V = 0$ $\therefore \frac{d^2\psi_3}{dx^2} + \frac{2mE}{\hbar^2}\psi_3 = 0$

$\therefore \psi_3(x) = Ee^{ik_1x} + Fe^{-ik_1x}$

1st term represents transimmitted wave. 2nd term represents reflected wave, but since at $x > a$ there is no sudden change in the Potential $\rightarrow$ we cannot have reflected wave back again $\rightarrow F = 0$

$$\therefore \psi(x) = \begin{cases} \psi_1(x) = A e^{ik_1 x} + B e^{-ik_1 x} \\ \psi_2(x) = C e^{ik_2 x} + D e^{-ik_2 x} \\ \psi_3(x) = E e^{ik_1 x} \end{cases}$$

By applying the boundary Conditions to find the Coefficients

1 - $\psi_1(x=0) = \psi_2(x=0)$

$\therefore A + B = C + D$ ①

2 - $\left.\frac{d\psi_1}{dx}\right|_{x=0} = \left.\frac{d\psi_2}{dx}\right|_{x=0}$

$\therefore ik_1 A - ik_1 B = ik_2 C - ik_2 D$

$\therefore k_1 (A - B) = k_2 (C - D)$ $\therefore A - B = \frac{k_2}{k_1}(C - D)$ ②

3 - $\psi_2(x=a) = \psi_3(x=a)$

$C e^{ik_2 a} + D e^{-ik_2 a} = E e^{ik_1 a}$ ③

4 - $\left.\frac{d\psi_2}{dx}\right|_{x=a} = \left.\frac{d\psi_3}{dx}\right|_{x=a}$

$\therefore ik_2 C e^{ik_2 a} - ik_2 D e^{-ik_2 a} = ik_1 E e^{ik_1 a}$

$\therefore Ce^{ik_2a} - De^{-ik_2a} = \frac{k_1}{k_2} Ee^{ik_1a}$ ④

add ① to ②

$2A_1 = C + D + \frac{k_2}{k_1}(C - D) = C + D + \frac{k_2}{k_1}C - \frac{k_2}{k_1}D$

$\therefore 2A_1 = C\left(1 + \frac{k_2}{k_1}\right) + D\left(1 - \frac{k_2}{k_1}\right)$ ⑤

Substract ① and ②

$2B = C + D - \frac{k_2}{k_1}C + \frac{k_2}{k_1}D \quad \therefore 2B = C\left(1 - \frac{k_2}{k_1}\right) + D\left(1 + \frac{k_2}{k_1}\right)$ ⑥

add ③ to ④

$2Ce^{ik_2a} = Ee^{ik_1a} + \frac{k_1}{k_2}Ee^{ik_1a} = Ee^{ik_1a}\left(1 + \frac{k_1}{k_2}\right)$

$\therefore C = \frac{1}{2}Ee^{ik_1a - ik_2a}\left(1 + \frac{k_1}{k_2}\right)$

$\therefore C = \frac{E}{2}e^{ia(k_1 - k_2)}\left(1 + \frac{k_1}{k_2}\right)$ ⑦

Substract ③ and ④

$2De^{-ik_2a} = Ee^{ik_1a} - \frac{k_1}{k_2}Ee^{ik_1a} = Ee^{ik_1a}\left(1 - \frac{k_1}{k_2}\right)$

$\therefore D = \frac{E}{2}e^{ia(k_1 + k_2)}\left(1 - \frac{k_1}{k_2}\right)$ ⑧

Subistitute from ⑦ & ⑧ in ⑤

$$\therefore 2A_1 = \frac{E}{2} e^{ia(k_1-k_2)}\left(1+\frac{k_1}{k_2}\right)\left(1+\frac{k_2}{k_1}\right) + \frac{E}{2} e^{ia(k_1+k_2)}\left(1-\frac{k_2}{k_1}\right)\left(1-\frac{k_2}{k_1}\right)$$

$$\left(1+\frac{k_1}{k_2}\right)\left(1+\frac{k_2}{k_1}\right) = 1+\frac{k_1}{k_2}+\frac{k_2}{k_1}+\frac{k_1k_2}{k_2k_1} = 2+\frac{k_1}{k_2}+\frac{k_2}{k_1}$$

$$,\left(1-\frac{k_2}{k_1}\right)\left(1-\frac{k_1}{k_2}\right) = 1+\frac{k_2k_1}{k_1k_2}-\frac{k_2}{k_1}-\frac{k_1}{k_2} = 2-\left(\frac{k_1}{k_2}+\frac{k_2}{k_1}\right)$$

$$\therefore A_1 = \frac{E}{4} e^{ia(k_1-k_2)}\left(2+\frac{k_1}{k_2}+\frac{k_2}{k_1}\right) + \frac{E}{4} e^{ia(k_1+k_2)}\left(2-\frac{k_1}{k_2}-\frac{k_2}{k_1}\right)$$

$$\therefore A = \frac{E}{4} e^{iak_1}\left[2e^{-iak_2}+\left(\frac{k_1}{k_2}+\frac{k_2}{k_1}\right)e^{-iak_2}+2e^{iak_2}-\left(\frac{k_1}{k_2}+\frac{k_2}{k_1}\right)e^{iak_2}\right]$$

$$\therefore A = \frac{E}{4} e^{iak_1}\left[2\left(e^{iak_2}+e^{-iak_2}\right)-\left(\frac{k_1}{k_2}+\frac{k_2}{k_1}\right)\left(e^{iak_2}-e^{-iak_2}\right)\right]$$

$$\therefore \cos\theta = \frac{e^{i\theta}+e^{-i\theta}}{2}, \quad \sin\theta = \frac{e^{i\theta}-e^{-i\theta}}{2i}$$

$$\therefore A = \frac{E}{4} e^{iak_1}\left[4\cos(ak_2) - 2i\sin(ak_2)\left(\frac{k_1}{k_2}+\frac{k_2}{k_1}\right)\right] \quad ⑨$$

The Transmission Coefficient T :

$$T = \left|\frac{E}{A}\right|^2$$

$$, \frac{E}{A} \therefore \left|\frac{A}{E}\right|^2 = \cos^2(ak_2) + \frac{1}{2}\sin^2(ak_2)\left(\frac{k_1^2+k_2^2}{k_1k_2}\right)^2$$

$\therefore \cos^2(ak_2) = 1 - \sin^2(ak_2)$

$\therefore \left|\frac{A}{E}\right|^2 = 1 - \sin^2(ak_2) + \left(\frac{k_1^2 + k_2^2}{2k_1k_2}\right)^2 \sin^2(ak_2)$

$\therefore \left|\frac{A}{E}\right|^2 = 1 + \left[\left(\frac{k_1^2 + k_2^2}{2k_1k_2}\right)^2 - 1\right] \sin^2(ak_2)$

$\frac{k_1^4 + 2k_1^2k_2^2 + k_2^4 - 4k_1^2k_2}{4k_1^2k_2^2} = \left(\frac{k_1^2 - k_2^2}{2k_1k_2}\right)^2$

$\therefore \left|\frac{A}{E}\right|^2 = 1 + \left(\frac{k_1^2 - k_2^2}{2k_1k_2}\right)^2 \sin^2(ak_2)$

$\therefore T = \left[1 + \left(\frac{k_1^2 - k_2^2}{2k_1k_2}\right) \sin^2(ak_2)\right]^{-1}$ (10)

Let $\varepsilon = \frac{E}{V_0}$, $\lambda = a\frac{\sqrt{2mV_0}}{\hbar}$

$\therefore \left(\frac{k_1^2 - k_2^2}{2k_1k_2}\right)^2 = \frac{(k_1^2 - k_2^2)^2}{4k_1^2k_2^2}$

$, k_1^2 - k_2^2 = \frac{2mE}{\hbar^2} - \frac{2m(E - V_0)}{\hbar^2} = \frac{2mV_0}{\hbar^2}$

$, 4k_1^2k_2^2 = 4\left(\frac{2mE}{\hbar^2}\right)\left(\frac{2m(E - V_0)}{\hbar^2}\right) = 4\left(\frac{2mV_0}{\hbar^2}\right)^2\left(\frac{E}{V_0}\right)\left(\frac{E}{V_0} - 1\right)$

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$$\therefore \frac{(K_1^2 - K_2^2)^2}{4K_1^2K_2^2} = \frac{1}{4\left(\frac{E}{V_0}\right)\left(\frac{E}{V_0}-1\right)} = \frac{1}{4\mathcal{E}(\mathcal{E}-1)} \quad (11)$$

$$\text{and } aK_2 = a\sqrt{\frac{2m(E-V_0)}{\hbar^2}} = a\sqrt{\frac{2mV_0}{\hbar^2}}\sqrt{\frac{E}{V_0}-1} = \lambda\sqrt{\mathcal{E}-1} \quad (12)$$

From (11) & (12) in (10)

$$\therefore T = \left[1 + \frac{1}{4\mathcal{E}(\mathcal{E}-1)}\sin^2(\lambda\sqrt{\mathcal{E}-1})\right]^{-1}$$

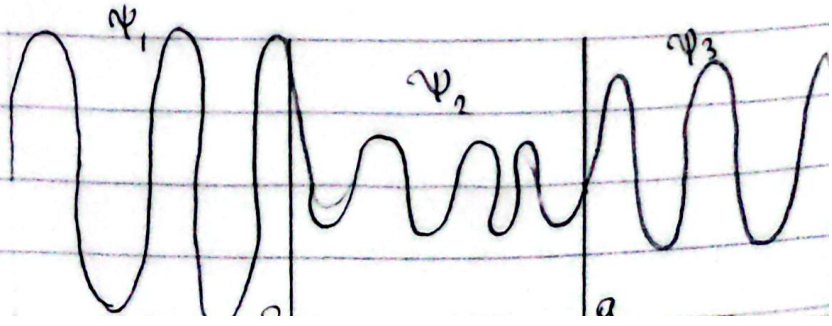
$$\text{or } R+T = 1 \quad \therefore R = 1-T$$

$$\therefore R = \left[1 + \frac{4\mathcal{E}(\mathcal{E}-1)}{\sin^2(\lambda\sqrt{\mathcal{E}-1})}\right]^{-1}$$

$$\therefore \boxed{T = \left[1 + \frac{1}{4\mathcal{E}(\mathcal{E}-1)}\sin^2(\lambda\sqrt{\mathcal{E}-1})\right]^{-1}}$$

$$\boxed{R = \left[1 + \frac{4\mathcal{E}(\mathcal{E}-1)}{\sin^2(\lambda\sqrt{\mathcal{E}-1})}\right]^{-1}}$$

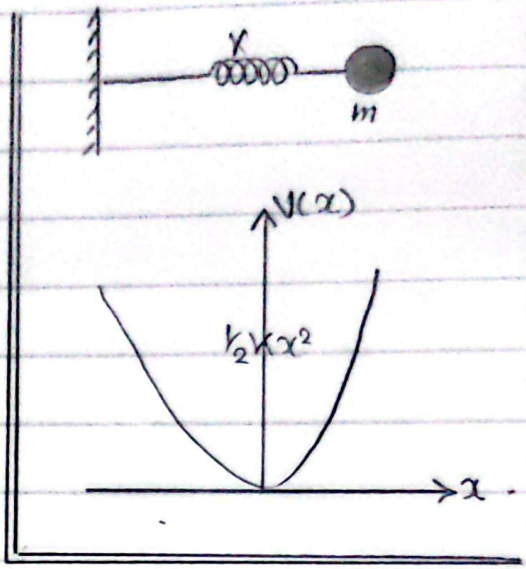
Even $E > V_0$ there is ____ which is different than classical mechanics.



4- The linear harmonic oscillator:

A classical linear harmonic oscillator consists of a particle of mass m subjected to a restoring force is given by

$$F = -kx$$



The potential energy associated with this force is

$$V(x) = -\int_0^x F(x)\,dx = -\int_0^x -kx\,dx$$

$$\therefore V(x) = \frac{1}{2}kx^2 \quad , \quad \because \omega = \sqrt{\frac{k}{m}} \quad \therefore V(x) = \frac{1}{2}m\omega^2 x^2$$

to determine the allowed quantum energy levels (E) and their corresponding stationary states wavefunctions $\psi(x)$:

TISE

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

$$\therefore \frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2\,\psi(x) = E\,\psi(x)$$

This equation is densely packed with dimensionful constants ($\hbar, m, \omega$), we define a dimensionless spatial variable z or ξ, and a dimensionless energy parameter, denoted by ε or K.

$$\text{let } z = \alpha x \quad \left(\alpha = \sqrt{\frac{m\omega}{\hbar}}\right) \rightarrow z = \sqrt{\frac{m\omega}{\hbar}}\,x \quad \therefore x^2 = \frac{\hbar}{m\omega}z^2$$

$$\therefore \frac{d\psi}{dx} = \frac{d\psi}{dz}\frac{dz}{dx} \quad , \frac{dz}{dx} = \sqrt{\frac{m\omega}{\hbar}}$$

$$\therefore \frac{d\psi}{dx} = \sqrt{\frac{m\omega}{\hbar}}\frac{d}{dz}$$

$$\frac{d^2\psi}{dx^2} = \frac{d}{dx}\left(\frac{d\psi}{dx}\right) = \frac{d}{d}\left(\sqrt{\frac{m\omega}{\hbar}}\frac{d\psi}{dz}\right)\frac{dz}{dx}$$

$$\therefore \frac{d^2\psi}{dx^2} = \sqrt{\frac{m\omega}{\hbar}}\left(\frac{d^2\psi}{dz^2}\sqrt{\frac{m\omega}{\hbar}}\right) = \frac{m\omega}{\hbar}\frac{d^2\psi}{dz^2}$$

Subistitute, x^2, $\frac{d^2\psi}{dx^2}$ into TISE

$$\therefore \frac{-\hbar^2}{2m}\left(\frac{m\omega}{\hbar}\frac{d^2\psi}{dz^2}\right) + \frac{1}{2}m\omega^2\frac{\hbar}{m\omega}z^2\psi = E\psi$$

$$\therefore \frac{-\hbar\omega}{2}\frac{d^2\psi}{dz^2} + \frac{\hbar\omega}{2}z^2\psi = E\psi \longrightarrow * \frac{-2}{\hbar\omega}$$

$$\therefore \frac{d^2\psi}{dz^2} - z^2\psi = \frac{-2E}{\hbar\omega}\psi \quad \therefore \frac{d^2\psi}{dz^2} + \left(\frac{2E}{\hbar\omega} - z^2\right)\psi = 0$$

Let $\varepsilon = \frac{2E}{\hbar\omega}$.

$$\therefore \frac{d^2\psi}{dz^2} + (\varepsilon - z^2)\psi = 0$$

We must examin the behavioral limits of the wave function at extreme distances, i.e $z \to \pm\infty$

Therefor $(\varepsilon - z^2) \to$ reducing to z^2

$$\therefore \frac{d^2\psi}{dz^2} - z^2\psi \simeq 0$$

and its solution is $\psi(z) = e^{\pm z^2/2}$

test the solution $\psi(z) \Rightarrow \frac{d\psi}{dz} = \pm z e^{\pm z^2/2}$

$$\frac{d^2\psi}{dz^2} = \pm 1 \cdot e^{\pm z^2/2} + (\pm z)(\pm z e^{z^2/2}) = (\pm 1 + z^2) e^{\pm z^2/2}$$

In the limit where $z \to \pm\infty \therefore (\pm 1 + z^2) \simeq z^2$

$$\therefore \frac{d^2\psi}{dz^2} \simeq z^2 e^{\pm z^2/2} = z^2\psi$$

The function $\psi(z)$ is vaild, but we need to know which behavior is right

$e^{z^2/2} \to$ grows exponentially without bound at $z \to \pm\infty$

$e^{-z^2/2} \to$ decays exponentially toward zero as $z \to \pm\infty$

from Born statistical interpretation $\int_{-\infty}^{\infty} |\psi|^2 dz = 1$

$\therefore e^{z^2/2} \to$ Cannot be normalized, so we will discard it

The proper Physical asymptotic function $f(z) = e^{-z^2/2}$

to form an exact solution, not approximated

Let $\psi(\tau) = u(\tau) f(\tau) = u(\tau)\, e^{-\tau^2/2}$

$u(\tau)$ accounts for the behavior near the center, $f(\tau) \rightarrow$ accounts at the boundary.

we need to substitute this ansatz into our exact eq.

$$\frac{d^2\psi}{d\tau^2} + (\varepsilon - \tau^2)\psi = 0$$

$$\therefore \frac{d\psi}{d\tau} = \frac{du}{d\tau} e^{-\tau^2/2} + u(\tau)(-\tau e^{-\tau^2/2})$$

$$\therefore \frac{d\psi}{d\tau} = \left(\frac{du}{d\tau} - \tau u(\tau)\right) e^{-\tau^2/2} \quad \textcircled{1}$$

$$\frac{d^2\psi}{d\tau^2} = \left[\frac{d^2u}{d\tau^2} - 2\tau\frac{du}{d\tau} + (\tau^2 - 1)u\right] e^{-\tau^2/2} \quad \textcircled{2}$$

Sub from 1 & 2 into TISE.

$$\therefore \left[\frac{d^2u}{d\tau^2} - 2\tau\frac{du}{d\tau} + (\tau^2 - 1)u\right] e^{-\tau^2/2} + (\varepsilon - \tau^2) u(\tau)\, e^{-\tau^2/2}$$

divide the equation by $e^{-\tau^2/2}$ since it cannot ever $= 0$

$$\therefore \frac{d^2u}{d\tau^2} - 2\tau\frac{du}{d\tau} + (\tau^2 - 1)u + (\varepsilon - \tau^2)u = 0$$

$$\therefore \frac{d^2u}{d\tau^2} - 2\tau\frac{du}{d\tau} + \tau^2 u - u + \varepsilon u - \tau^2 u = 0$$

$$\therefore \frac{d^2u}{d\tau^2} - 2\tau\frac{du}{d\tau} - u + \varepsilon u = 0$$

$$\therefore \frac{d^2u}{d\tau^2} - 2\tau \frac{du}{d\tau} + (\varepsilon - 1)u = 0$$

Right now we want to solve this differential equation It can be solved via Power series like in Griffith or using an easy method, which is one of the special function.

$$\therefore \frac{d^2u}{d\tau^2} - 2\tau \frac{du}{d\tau} + (\varepsilon - 1)u = 0$$

and Hermite function

$$H_n'' - 2x H_n' + 2n H_n = 0$$

by Comparing these two diff. equ.

$$\therefore u(\tau) = H_n(\tau) \quad , \quad 2n = \varepsilon - 1 \quad \therefore 2n = \frac{2E}{\hbar\omega} - 1$$

$$\therefore \frac{2E}{\hbar\omega} = 2n + 1 \quad \therefore 2E = \hbar\omega(2n+1)$$

$$\therefore \boxed{E = \hbar\omega\left(n + \frac{1}{2}\right)} \qquad n = 0, 1, 2, 3, \ldots$$

Constructing the wavefunction via Hermite Polynomials.

$$\therefore u(\tau) = H_n(\tau) \quad \therefore \psi_n(\tau) = H_n(\tau)\, e^{-\tau^2/2}$$

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for Ground state : $n=0$: $H_0(z)=a_0$
1st excited state : $n=1$: $H_1(z)=2z$
2nd excited state : $n=2$: $H_2(z)=4z^2-2$

We must find the normalization Constant

$$\int_{-\infty}^{\infty}|\psi_n(x)|^2dx=1 \longrightarrow \int_{-\infty}^{\infty}\left|N_n H_n(z)e^{-z^2/2}\right|^2 dx=1$$

$$\therefore z=\sqrt{\frac{m\omega}{\hbar}}\,x \quad \therefore dx=\sqrt{\frac{\hbar}{m\omega}}\,dz$$

$$\therefore |N_n|^2\sqrt{\frac{\hbar}{m\omega}}\int_{-\infty}^{\infty}[H_n(z)]^2 e^{-z^2}dz=1$$

$$\therefore \int_{-\infty}^{\infty}[H_n(z)]^2 e^{-z^2/2}dz=2^n n!\sqrt{\pi}$$ from orthogonal properties of Hermit Polynomials using Rodrigues Formula and Integration by Parts.

$$\therefore |N_n|^2\sqrt{\frac{\hbar}{m\omega}}\cdot 2^n n!\sqrt{\pi}=1 \quad \therefore |N_n|^2=\sqrt{\frac{m\omega}{\hbar}}\,\frac{1}{2^n n!\sqrt{\pi}}$$

α

$$\therefore N_n=\left(\frac{m\omega}{\hbar\pi}\right)^{1/4}\frac{1}{\sqrt{2^n n!}} \qquad |N_n|^2=\frac{\alpha}{2^n n!\sqrt{\pi}}$$

$$\therefore N=\frac{\alpha}{2^n n!\sqrt{\pi}}$$

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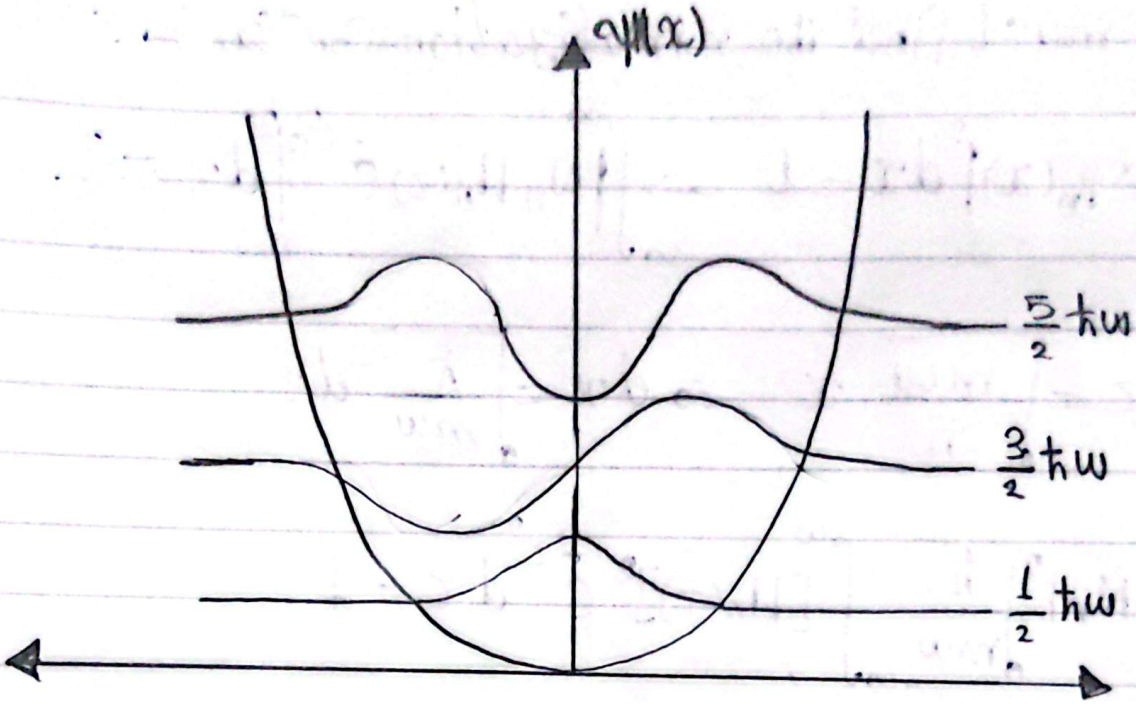
$$\therefore \boxed{\psi_n(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}\, x\right) e^{-\frac{m\omega}{2\hbar}x^2}}$$



Comments:

1_ In classical mechanics, the harmonic oscillator can absorb or release any continous amount of energy, But in QM it gives a discrete energy spectrum.

2_ In classical mechanics, the abslute lowest energy state of an oscillator $n=0$ has $E=0$, but in QM $E = \frac{1}{2}\hbar\omega$.

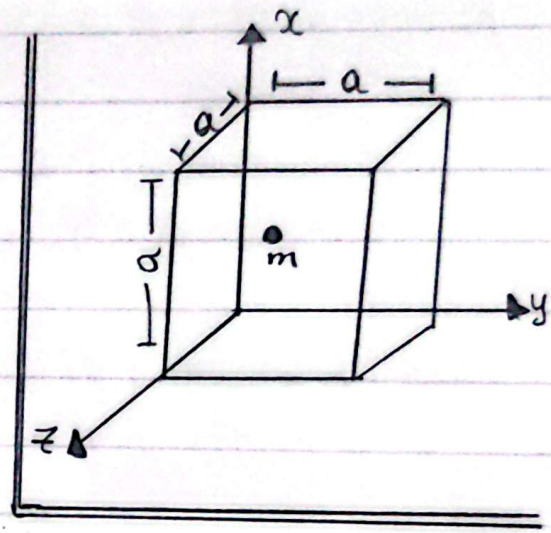
Lecture (5) 6/7/2026

Three Dimensional Problems

1- The Cubic Box Potential:

Considre a Pantide of mass m held in a cubic box with side length a under no Potential inside the box:

$$V(x,y,z) = \begin{cases} 0 & \text{if } 0<x<a \\ & 0<y<a \\ & 0<z<a \\ \infty & \text{otherwise} \end{cases}$$



Solution of this problem

TISE

$$\frac{-\hbar^2}{2m}\nabla^2\psi(x,y,z) + V\psi = E\psi$$

$\because V = 0$ inside the box , $\therefore \frac{-\hbar^2}{2m}\nabla^2\psi = E\psi$

$$\frac{-\hbar}{2m}\left[\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right] = E\psi(x,y,z)$$

Using seperation of Variables method to Solve this diff- erential equation :

$$\psi(x,y,z) = X(x)\,Y(y)\,Z(z)$$

$$\therefore \frac{\partial^2\psi}{\partial x^2} = YZ\frac{d^2X}{dx^2} \quad , \quad \frac{\partial^2\psi}{\partial y^2} = XZ\frac{d^2Y}{dy^2} \quad , \quad \frac{\partial^2\psi}{\partial z^2} = XY\frac{d^2Z}{dz^2}$$

$$\therefore YZ\frac{d^2X}{dx^2} + XZ\frac{d^2Y}{dy^2} + XY\frac{d^2Z}{dz^2} = \frac{-2m}{\hbar^2} E XYZ$$

divide both sides by XYZ

$$\therefore \frac{1}{X}\frac{d^2X}{dx^2} + \frac{1}{Y}\frac{d^2Y}{dy^2} + \frac{1}{Z}\frac{d^2Z}{dz^2} = \frac{-2mE}{\hbar^2}$$

Let : $\frac{1}{X}\frac{d^2X}{dx^2} = -K_x^2$ $\therefore \frac{d^2X}{dx^2} + K_x^2 X = 0$

$\therefore X(x) = C_1 \sin(K_x x) + C_2 \cos(K_x x)$

by applying the boundary Conditions :

1 - $X(x=0) = 0$ $\therefore C_1(0) + C_2(1) = 0$

$\therefore C_2 = 0$

$\therefore X(x) = C_1 \sin(K_x x)$

2 - $X(x=a) = 0$ $\therefore C_1 \sin(K_x a) = 0$

$\therefore K_x a = n_x \pi$

$\therefore K_x = \frac{n_x \pi}{a}$

$\therefore X(x) = C_1 \sin\left(\frac{n_x \pi}{a} x\right)$ (1) eigenfunction solution around x-axis.

Let : $\frac{1}{Y}\frac{d^2Y}{dy^2} = -K_y^2$ $\therefore \frac{d^2Y}{dy^2} + K_y^2 Y = 0$

$\therefore Y(y) = C_3 \sin(K_y y) + C_4 \cos(K_y y)$

by applying the boundary Conditions :

3 - $Y(y=0) = 0$

$\therefore C_3(0) + C_4(1) = 0$ $\therefore C_4 = 0$

4- $Y(y=a) = 0$ $\therefore C_3 \sin(k_y a) = 0$

$\therefore k_y a = n_y \pi$ $\therefore k_y = \frac{n_y \pi}{a}$

$\therefore Y(y) = C_3 \sin\left(\frac{n_y \pi}{a} y\right)$ ② eigenfunction solution around y-axis

Let $\frac{1}{Z}\frac{d^2Z}{dz^2} = -k_z^2$ $\therefore \frac{d^2Z}{dz^2} + k_z^2 Z = 0$

$\therefore Z(z) = C_5 \sin(k_z a) + C_6 \cos(k_z a)$

by applying the boundary conditions:

5- $Z(z=0) = 0$ $\therefore C_5(0) + C_6(1) = 0 \rightarrow C_6 = 0$

6- $Z(z=a) = 0$ $\therefore C_5 \sin(k_z a) = 0$

$\therefore k_z a = n_z \pi$ $\therefore k_z = \frac{n_z \pi}{a}$

$\therefore Z(z) = C_5 \sin\left(\frac{n_z \pi}{a} z\right)$

$\therefore \psi(x,y,z) = C_1 C_3 C_5 \sin\left(\frac{n_x \pi}{a} x\right) \sin\left(\frac{n_y \pi}{a} y\right) \sin\left(\frac{n_z \pi}{a} z\right)$

to find these coeffecients C_1, C_3 and C_5 we have to normalize the function.

Normalization: $\iiint \psi^*(x,y,z)\, \psi(x,y,z)$

$$\therefore \int_V |\psi|^2 dV = 1$$

$$\therefore (C_1C_3C_5)^2 \int_0^a \sin^2\left(\frac{n_x\pi}{a}x\right)dx \int_0^a \sin^2\left(\frac{n_y\pi}{a}y\right)dy \int_0^a \sin\left(\frac{n_z\pi}{a}z\right)dz = 1$$

$$\because \sin^2\theta = \frac{1}{2}(1-\cos 2\theta)$$

$$\therefore (C_1C_3C_5)^2 \cdot \frac{1}{2}\int_0^a \left[1-\cos\left(\frac{2n_x\pi}{a}x\right)\right]dx \cdot \frac{1}{2}\int_0^a \left[1-\cos\left(\frac{2n_y\pi}{a}y\right)\right]dy$$

$$\cdot \frac{1}{2}\int_0^a \left[1-\cos\left(\frac{2n_z\pi}{a}z\right)\right]dz = 1$$

$$\therefore (C_1C_3C_5)^2 \cdot \frac{1}{8}\left[x - \frac{a}{2n_x\pi}\sin\left(\frac{2n_x\pi}{a}x\right)\right]_0^a$$

$$\left[y - \frac{a}{2n_y\pi}\sin\left(\frac{2n_y\pi}{a}y\right)\right]_0^a \left[z - \frac{a}{2n_z\pi}\sin\left(\frac{2n_z\pi}{a}z\right)\right]_0^a = 1$$

$$\because \sin\left(\frac{2n_y\pi}{a}y\right)\Big|_0^a = \sin(2n_y\pi) = 0$$

$$\therefore (C_1C_3C_5)^2 \cdot \frac{1}{8}[a-0][a-0][a-0] = 1$$

$$\therefore (C_1C_3C_5)^2 = \frac{8}{a^3} \quad \therefore C_1C_3C_5 = \sqrt{\frac{8}{a^3}}$$

$$\therefore C_1 = C_3 = C_5 = \sqrt{\frac{2}{a}}$$

$$\therefore \boxed{\psi(x,y,z) = \sqrt{\frac{2}{a}}\sin\left(\frac{n_x\pi}{a}x\right)\sqrt{\frac{2}{a}}\sin\left(\frac{n_y\pi}{a}y\right)\sqrt{\frac{2}{a}}\sin\left(\frac{n_z\pi}{a}z\right)}$$

→ Eigenfunction Solution of Cubic Potential well:

n_x, n_y, n_z : Quantum numbers associated with eigenfunctions solutions around x, y, z-axis.

TDSE : $\psi(x,y,z,t) = \psi(x,y,z)\, e^{-iEt/\hbar}$

The energy levels :

$$\therefore \frac{1}{X}\frac{d^2X}{dx^2} + \frac{1}{Y}\frac{d^2Y}{dy^2} + \frac{1}{Z}\frac{d^2Z}{dz^2} = \frac{-2mE}{\hbar^2}$$

$$\therefore -(k_x^2 + k_y^2 + k_z^2) = \frac{-2mE}{\hbar^2}$$

$$\therefore \left(\frac{n_x \pi}{a}\right)^2 \left(\frac{n_y \pi}{a}\right)^2 \left(\frac{n_z \pi}{a}\right)^2 = \frac{2mE}{\hbar^2}$$

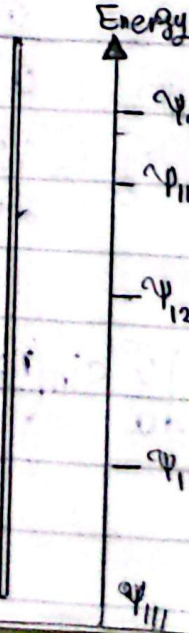
$$\therefore \left(\frac{\pi}{a}\right)^2 (n_x^2 + n_y^2 + n_z^2) = \frac{2mE}{\hbar^2}$$

$$\therefore \boxed{E_{n_x n_y n_z} = \frac{1}{2m}\left(\frac{\pi\hbar}{a}\right)^2 (n_x^2 + n_y^2 + n_z^2)}$$

↳ Energy levels associated with the eigenstates.

$\psi_{112}, \psi_{121}, \psi_{211}$ are eigenstates solutions having their own distinct Probability density, But Share the Same energy Level.

That's what we Call it degeneracy "eigenstates having the same energy value"



Another Cases:

1 _ If the Potential inside the box is V_0, and outside ∞.

$$\frac{-\hbar^2}{2m}\nabla^2\psi + V_0\psi = E\psi$$

The wave function will be the same:

$$\psi(x,y,z) = \sqrt{\frac{2}{a}}\sin\left(\frac{n_x\pi}{a}x\right)\sqrt{\frac{2}{a}}\sin\left(\frac{n_y\pi}{a}y\right)\sqrt{\frac{2}{a}}\sin\left(\frac{n_z}{a}z\right)$$

but:

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} = \frac{-2m}{\hbar}(E - V_0)$$

Then we will have

$$\boxed{E_{n_x,n_y,n_z} = V_0 + \frac{1}{2m}\left(\frac{\pi\hbar}{a}\right)^2(n_x^2 + n_y^2 + n_z^2)}$$

2 _ If The box was rectangular with side Length a, b, c for x, y, z _ axis:, and the particle is free inside the box.

$$\psi(x,y,z) = \sqrt{\frac{2}{a}}\sin\left(\frac{n_x\pi}{a}x\right)\sqrt{\frac{2}{b}}\sin\left(\frac{n_y\pi}{b}y\right)\sqrt{\frac{2}{c}}\sin\left(\frac{n_z\pi}{c}z\right)$$

$$E_{n_x,n_y,n_z} = \left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right)\frac{\pi^2\hbar^2}{2m}$$

لو مش حو هنزود ع الطاقة الجهد بس

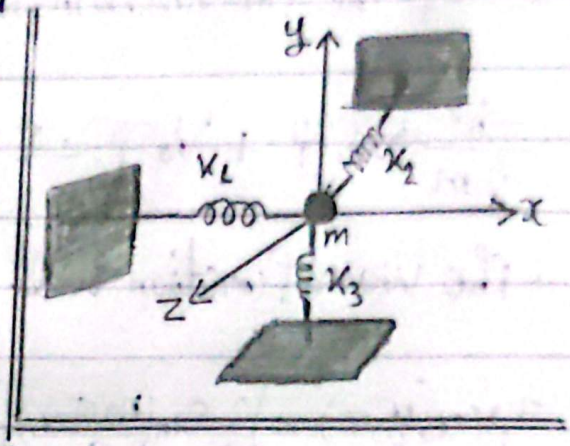
2- The Quantum Harmonic Anisotropic Oscillator:

المتذبذب التوافقي غير المتماثل

Considre a Particle of mass m moving in a 3D Anisotropic oscillator Potential:

$V(x,y,z) = \frac{1}{2}m(\omega_1^2x^2+\omega_2^2y^2+\omega_3^2z^2)$

or: $V(x,y,z) = \frac{1}{2}k_1x + \frac{1}{2}k_2y + \frac{1}{2}k_3z$



Solution:

TISE:

$$\frac{-\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

$$\therefore \frac{-\hbar^2}{2m}\nabla^2\psi + \frac{1}{2}m(\omega_1^2x^2+\omega_2^2y^2+\omega_3^2z^2)\psi = E\psi$$

using the method of separation of variables

$$\psi(x,y,z) = X(x)Y(y)Z(z)$$

$$\therefore \frac{-\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}\xrightarrow{}YZX + \frac{\partial^2\psi}{\partial y^2}\xrightarrow{}XZY + \frac{\partial^2\psi}{\partial z^2}\xrightarrow{}XYZ\right) + \frac{1}{2}m\omega_1^2x^2XYZ + \frac{1}{2}m\omega_2^2y^2XYZ + \frac{1}{2}m\omega_3^2z^2XYZ = EXYZ$$

$$\therefore \frac{-\hbar^2}{2m}\left[YZ\frac{d^2X}{dx^2} + XZ\frac{d^2Y}{dy^2} + XY\frac{d^2Z}{dz^2}\right] + \frac{1}{2}m\omega_1^2x^2XYZ + \frac{1}{2}m\omega_2^2y^2XYZ + \frac{1}{2}m\omega_3^2z^2XYZ = EXYZ$$

divide the entire equation by XYZ

$$\therefore \left[\frac{-\hbar^2}{2m}\frac{1}{X}\frac{d^2X}{dx^2} + \frac{1}{2}m\omega_1^2x^2\right] + \left[\frac{-\hbar^2}{2m}\frac{1}{Y}\frac{d^2Y}{dy^2} + \frac{1}{2}m\omega_2^2y^2\right] + \left[\frac{-\hbar^2}{2m}\frac{1}{Z}\frac{d^2Z}{dz^2} + \frac{1}{2}m\omega_3^2\right] = E$$

These bracketed terms are respectively functions of x only, y only, z only — and their sum is a constant E. So each bracketed term should be to a constant.

$$\frac{-\hbar^2}{2m}\frac{1}{X}\frac{d^2X}{dx^2} + \frac{1}{2}m\omega_1^2x^2 = E_x \quad (1)$$

$$\frac{-\hbar^2}{2m}\frac{1}{Y}\frac{d^2Y}{dy^2} + \frac{1}{2}m\omega_2^2y^2 = E_y \quad (2)$$

$$\frac{-\hbar^2}{2m}\frac{1}{Z}\frac{d^2Z}{dz^2} + \frac{1}{2}m\omega_3^2z^2 = E_z \quad (3)$$

This gives rise to three ordinary 1-D differential equation.

Solution of x-axis:

$$\frac{-\hbar^2}{2m}\frac{d^2X}{dx^2} + \frac{1}{2}m\omega_1^2x^2X = E_xX$$

Let; $\alpha^2 = \frac{m\omega_1}{\hbar}$ $\therefore \alpha = \sqrt{\frac{m\omega_1}{\hbar}}$, $\xi = \alpha x$

$\therefore \frac{dX}{dx} = \frac{dX}{d\xi}\frac{d\xi}{dx}$, $\frac{d\xi}{dx} = \alpha = \sqrt{\frac{m\omega_1}{\hbar}}$

$\therefore \frac{dX}{dx} = \sqrt{\frac{m\omega_1}{\hbar}}\frac{dX}{d\xi}$ $\therefore \frac{d^2X}{dx^2} = \frac{m\omega_1}{\hbar}\frac{d^2X}{d\xi^2}$

$\therefore x^2 = \frac{\xi^2}{\alpha^2}$, Sub. from $\frac{d^2X}{dx^2}$, x^2 into the D.E

$\therefore \frac{-\hbar^2}{2m}\left(\frac{m\omega_1}{\hbar}\frac{d^2X}{d\xi^2}\right) + \frac{1}{2}m\omega_1^2\left(\frac{\xi^2}{\alpha^2}\right)X = E_x X$

$\hookrightarrow \alpha = \sqrt{\frac{m\omega_1}{\hbar}}$

$\therefore \frac{-\hbar}{2}\omega_1\frac{d^2X}{d\xi^2} + \frac{1}{2}m\omega_1^2\left(\frac{\hbar\xi^2}{m\omega_1}\right)X = E_x X$

$\therefore \frac{-\hbar}{2}\omega_1\frac{d^2X}{d\xi^2} + \frac{1}{2}\hbar\omega_1\xi^2 X = E_x X \quad * \frac{-2}{\hbar\omega_1}$

$\therefore \frac{d^2X}{d\xi^2} - \xi^2 X = \frac{-2E_x}{\hbar\omega_1}X$, let $\varepsilon_1 = \frac{2E_x}{\hbar\omega_1}$

$\therefore \frac{d^2X}{d\xi^2} - \xi^2 X + \varepsilon_1 X = 0 \quad \therefore \frac{d^2X}{d\xi^2} + (\varepsilon_1 - \xi^2)X = 0$ (1)

This D.E has Solution of $X(\xi) = e^{-\xi^2/2}$

to form exact solution, not approximated

let $X(\xi) = u(\xi)e^{-\xi^2/2}$, subistitute this ansatz

in $\frac{d^2X}{d\xi^2} + (\varepsilon_1 - \xi^2)X = 0$

$\therefore \frac{dX}{d\xi} = \frac{du}{d\xi}e^{-\xi^2/2} + u(\xi)(-\xi e^{-\xi^2/2})$

$$\therefore \frac{dX}{d\xi} = \left(\frac{du}{d\xi} - u(\xi)\xi\right) e^{-\xi^2/2} \quad \text{②}$$

$$\frac{d^2X}{d\xi^2} = \frac{d^2u}{d\xi^2} - 2\xi\frac{du}{d\xi} + (\xi^2 - 1)u\Big] e^{-\xi^2/2} \quad \text{③}$$

Sub from ② & ③ in ①

$$\therefore \left[\frac{d^2u}{d\xi^2} - 2\xi\frac{du}{d\xi} + (\xi^2 - 1)u\right] e^{-\xi^2/2} + (\varepsilon_1 - \xi^2)u\, e^{-\xi^2/2} = 0$$

divide the entire equation by $e^{-\xi^2/2}$

$$\therefore \frac{d^2u}{d\xi^2} - 2\xi\frac{du}{d\xi} + (\xi^2 - 1)u + (\varepsilon_1 - \xi^2)u = 0$$

$$\therefore \frac{d^2u}{d\xi^2} - 2\xi\frac{du}{d\xi} + \xi^2 u - u + \varepsilon_1 u - \xi^2 u = 0$$

$$\therefore \frac{d^2u}{d\xi^2} - 2\xi\frac{du}{d\xi} + (\varepsilon_1 - 1)u = 0 \quad \text{④}$$

Using Hermite function; $H_n'' - 2xH_n' + 2nH_n = 0$ ⑤

Compare ④ & ⑤

$$\therefore \varepsilon_1 - 1 = 2n_1 \qquad \therefore \varepsilon_1 = 2n_1 + 1 \;, \quad \because \varepsilon_1 = \frac{2E_x}{\hbar\omega_1}$$

$\therefore 2n_1 + 1 = \frac{2E_x}{\hbar\omega_1} \quad \therefore E_x = \hbar\omega_1\left(n_1 + \frac{1}{2}\right)$

by the same steps we can evaluate E_y, E_z

$E_y = \hbar\omega_2\left(n_2 + \frac{1}{2}\right) \qquad E_z = \hbar\omega_3\left(n_3 + \frac{1}{2}\right)$

Then the 'Eigenvalues' for 3D oscillator is the sum of E_x, E_y and E_z.

$$\therefore \boxed{E_{n_1,n_2,n_3} = \hbar\omega_1\left(n_1 + \tfrac{1}{2}\right) + \hbar\omega_2\left(n_2 + \tfrac{1}{2}\right) + \hbar\omega_3\left(n_3 + \tfrac{1}{2}\right)}$$

to find the wave function around x-axis

$$\therefore u(\xi) = H_n(\xi) \quad \therefore X(\xi) = H_{n_1}(\xi)\, e^{-\xi^2/2}$$

to find the normalization constant:

$$\int_{-\infty}^{\infty} |\psi^* \psi \, dx\, dy\, dz = 1 \quad \therefore \int_{-\infty}^{\infty} |X|^2 \, dx = 1$$

$$\therefore \int_{-\infty}^{\infty} \left| N_{n_1} H_n(\xi)\, e^{-\xi^2/2} \right|^2 dx = 1 \quad , \quad \therefore \xi = \sqrt{\frac{m\omega_1}{\hbar}}\, x$$

$$\therefore dx = \sqrt{\frac{\hbar}{m\omega_1}}\, d\xi$$

$$\therefore |N_{n_1}|^2 \sqrt{\frac{\hbar}{m\omega_1}} \int_{-\infty}^{\infty} [H_n(\xi)]^2 e^{-\xi^2/2} d\xi = 1$$

$$\therefore \int_{-\infty}^{\infty} [H_n(\xi)]^2 e^{-\xi^2/2} d\xi = 2^n n_1! \sqrt{\pi}$$

$$\therefore |N_{n_1}|^2 \sqrt{\frac{\hbar}{m\omega_1}} \cdot 2^{n_1} n_1! \sqrt{\pi} = 1$$

$$\therefore |N_{n_1}|^2 = \frac{\alpha_1}{2^{n_1} n_1! \sqrt{\pi}} \qquad \therefore N_{n_1} = \sqrt{\frac{\alpha_1}{2^{n_1} n_1! \sqrt{\pi}}}$$

The same normalization process for $Y(y)$ and $Z(z)$

$$\therefore N_{n_2} = \sqrt{\frac{\alpha_2}{2^{n_2} n_2! \sqrt{\pi}}}, \quad N_{n_3} = \sqrt{\frac{\alpha_3}{2^{n_3} n_3! \sqrt{\pi}}}$$

$\therefore$ The eigenfunction will be the product of three 1D oscillator eigen wave function.

$$\psi_{n_1,n_2,n_3} = N_{n_1} N_{n_2} N_{n_3} e^{-\frac{1}{2}(\xi_1^2 + \xi_2^2 + \xi_3^2)} H_{n_1}(\xi_1) H_{n_2}(\xi_2) H_{n_3}(\xi_3)$$

$$\therefore \boxed{\psi_{n_1,n_2,n_3}(x,y,z) = \left(\frac{\alpha_1 \alpha_2 \alpha_3}{2^{(n_1+n_2+n_3)} n_1! n_2! n_3!} \right)^{1/2} e^{-\frac{1}{2}(\xi_1^2 + \xi_2^2 + \xi_3^2)} H_{n_1}(\xi_1) H_{n_2}(\xi_2) H_{n_3}(\xi_3)}$$

$\rightarrow$ eigen functions.

For an Isotropic oscillator force constant (k_1, k_2, k_3) and hence frequencies $(\omega_1, \omega_2, \omega_3)$ are the same along the three axis.

$$k_1 = k_2 = k_3 \quad \therefore \omega_1 = \omega_2 = \omega_3$$

$$\therefore E_{n_1, n_2, n_3} = \hbar\omega\left(n_1 + n_2 + n_3 + \frac{3}{2}\right)$$

$$\psi_{n_1, n_2, n_3}(x, y, z) = \sqrt{\frac{\alpha^3}{2^{n_1+n_2+n_3} n_1! n_2! n_3! \pi^{3/2}}}\, e^{-\frac{1}{2}\alpha^2(x^2+y^2+z^2)} H_{n_1} H_{n_2} H_{n_3}$$

Let: $n = n_1 + n_2 + n_3$, $x^2 + y^2 + z^2 = r^2$

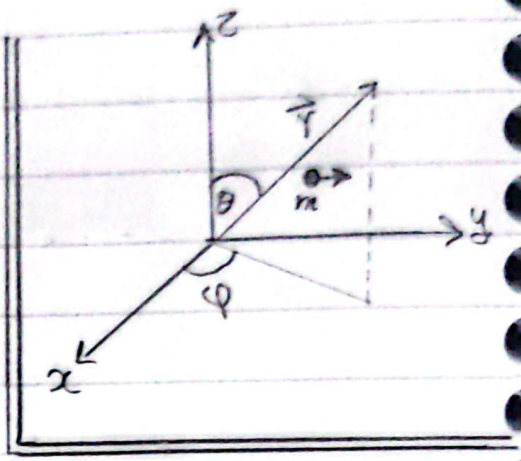
$$\therefore \psi_{n_1, n_2, n_3}(x, y, z) = \sqrt{\frac{\alpha^3}{2^n n_1! n_2! n_3! \pi^{3/2}}}\, e^{-\frac{1}{2}\alpha^2 r^2} H_{n_1} H_{n_2} H_{n_3}$$

Lecture (6) 6/10/2026

Three-Dimensional Problems

1- Quantum Treatment of Central Potentials:

Considre a particle of mass m moving in a central potential V(r) which means that the potential energy depends only on the radial distance, from the origin and has no angular dependance.



TISE:

$$\frac{-\hbar^2}{2m}\vec{\nabla}^2\psi + V(r)\psi = E\psi$$

$\vec{\nabla}^2$ in Spherical Coordinates:

$$\vec{\nabla}^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}$$

∴ TISE:

$$\therefore \frac{-\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2}\right] + V(r)\psi = E\psi$$

Let: $\psi(r,\theta,\varphi) = R(r)\,\Theta(\theta)\,\Phi(\varphi)$

$$\therefore \frac{-\hbar^2}{2m}\left[\frac{\Theta\Phi}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{R\Phi}{r^2\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \frac{R\Theta}{r^2\sin^2\theta}\frac{d^2\Phi}{d\varphi}\right] + V(r)R\Theta\Phi = E R\Theta\Phi$$

divide the entire equation by $R(r)\Theta(\theta)\Phi(\varphi)$

$$\therefore \left[\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\theta}{d\theta}\right)+\frac{1}{\Phi\sin^2\theta}\frac{d^2\Phi}{d\varphi}\right]+ = \frac{-2m}{\hbar^2}E$$

$$\therefore \underbrace{\left[\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-\frac{2m}{\hbar^2}(V(r)-E)\right]}_{1st}+\underbrace{\left[\frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\theta}{d\theta}\right)+\frac{1}{\Phi\sin^2\theta}\frac{d^2\Phi}{d\varphi^2}\right]}_{2nd} = 0$$

1st term depends only on r, 2nd term depends only on the angles θ and φ. Therefore each term equal a constant. Let the constant be λ

$$\therefore \frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-\frac{2m}{\hbar^2}(V(r)-E)=\lambda$$

$$, \frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\theta}{d\theta}\right)+\frac{1}{\Phi\sin^2\theta}\frac{d^2\Phi}{d\varphi^2}=-\lambda$$

multiply both sides by $\sin^2\theta$:

$$\frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\theta}{d\theta}\right)+\frac{1}{\Phi}\frac{d^2\Phi}{d\varphi^2}=-\lambda\sin^2\theta$$

$$\therefore \frac{-1}{\Phi}\frac{d^2\Phi}{d\varphi^2}=\frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\theta}{d\theta}\right)+\lambda\sin^2\theta$$

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Left term: depends only on φ, Right term depends only on θ Therefore each one equal a constant

$$\frac{1}{\Phi}\frac{d\Phi^2}{d\varphi} = -m^2 \rightarrow \text{The "Azimuthal" equation}$$

$$\therefore \frac{d\Phi^2}{d\varphi} = m^2\Phi \quad \therefore \Phi(\varphi) = Ae^{\pm im\varphi} \quad , m = 0, \pm 1, \dots$$

to find the normalization coefficient of azimuthal part

$$\int_0^{2\pi} |\Phi|^2 d\varphi = 1 \quad \therefore A^2 \int_0^{2\pi} e^{-im\varphi} e^{+im\varphi} d\varphi = 1$$

$$\int_{-\infty}^{\infty} \psi^* \psi \, dV$$

$$\therefore A^2 \int_0^{2\pi} d\varphi = 1 \quad \therefore A^2 = \frac{1}{2\pi} \quad \therefore A = \frac{1}{\sqrt{2\pi}}$$

$$\therefore \boxed{\Phi(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi}} \rightarrow \text{Azimuthal Function, doesn't depend on } V(r)..$$

Polar equation: $\frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta \frac{d\theta}{d\theta}\right) + \lambda \sin^2\theta = m^2$

divide both sides by $\sin^2\theta$

$$\frac{1}{\Theta \sin\theta}\frac{d}{d\theta}\left(\sin\theta \frac{d\theta}{d\theta}\right) + \lambda = \frac{m^2}{\sin^2\theta}$$

, $\lambda = l(l+1)$

$$\therefore \frac{1}{\Theta \sin\theta}\frac{d}{d\theta}\left(\sin\theta \frac{d\Theta}{d\theta}\right) + \left[l(l+1) - \frac{m^2}{\sin^2\theta}\right]\Theta = 0$$

Put $x = 1 - \sin^2\theta = \cos^2\theta$

$$\therefore \frac{d}{dx}\left[(1-x^2)\frac{d\Theta}{dx}\right] + \left[l(l+1) - \frac{m^2}{1-x^2}\right]\Theta = 0 \quad (1)$$

Since the associated legendre differential equation:

$$\frac{d}{dx}\left[(1-x^2)\frac{dP_l^m}{dx}\right] + \left[l(l+1) - \frac{m^2}{1-x^2}\right]P_l^m(x) = 0 \quad (2)$$

Compare 1 & 2

$$\therefore \Theta_{lm} = A_l P_l^m(\cos\theta) \quad , l = 0, 1, 2$$

normalize Θ_{lm}

$$\therefore \Theta_{lm}(\theta) = (-1)^m \sqrt{\frac{(2l+1)(l-|m|)!}{2(l+|m|)!}}\, P_l^m(\cos\theta)$$

The full angular wavefunction:

$$Y_{lm_l}(\theta,\varphi) = \Theta(\theta)\Phi(\varphi)$$

$$\therefore \boxed{Y_{lm_l}(\theta,\varphi) = (-1)^m \sqrt{\frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!}}\, P_l^m(\cos\theta)\, e^{im\varphi}}$$

→ Spherical Harmonic Functions